

10/513699

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STRUCTURE FILE UPDATES: 27 FEB 2009 HIGHEST RN 1113101-98-6
DICTIONARY FILE UPDATES: 27 FEB 2009 HIGHEST RN 1113101-98-6

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

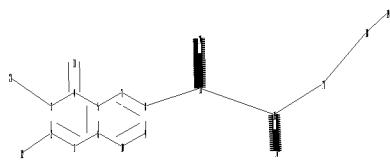
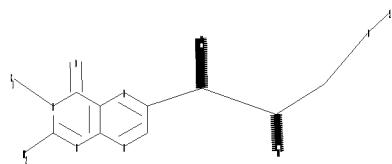
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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>
Uploading C:\Program Files\Stnexp\Queries\10579106restriction.str

10/513699



chain nodes :

11 12 13 14 15 16 17 18 19 21

ring nodes :

1 2 3 4 5 6 7 8 9 10

chain bonds :

2-12 3-21 4-11 8-13 13-14 13-15 15-16 15-17 17-18 18-19

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10

exact/norm bonds :

1-2 1-6 2-3 2-12 3-4 3-21 4-5 4-11 13-14 15-16 17-18

exact bonds :

8-13 13-15 15-17 18-19

normalized bonds :

5-6 5-7 6-10 7-8 8-9 9-10

isolated ring systems :

containing 1 :

G1:C,H

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 21:CLASS

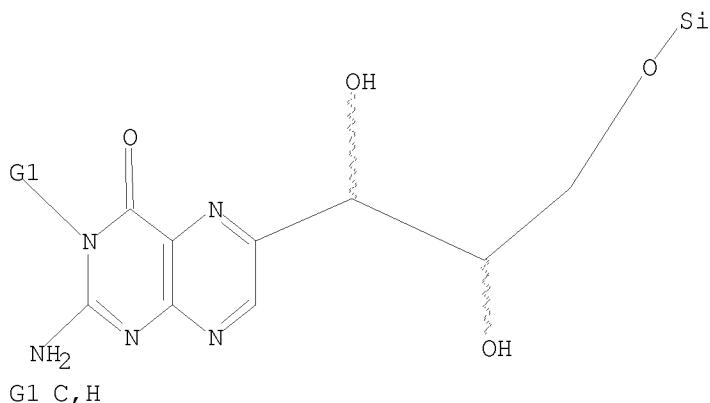
L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

10/513699



Structure attributes must be viewed using STN Express query preparation.

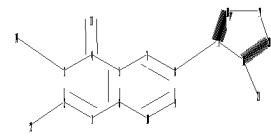
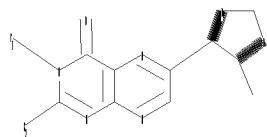
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SAMPLE SCREEN SEARCH COMPLETED -          2 TO ITERATE

100.0% PROCESSED      2 ITERATIONS          0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:      2 TO      124
PROJECTED ANSWERS:          0 TO      0

L2          0 SEA SSS SAM L1

=>
Uploading C:\Program Files\Stnexp\Queries\10579106ring.str
```



chain nodes :

11 12 14 21

ring nodes :

1 2 3 4 5 6 7 8 9 10 16 17 18 19 20

chain bonds :

2-12 3-14 4-11 8-17 16-21

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-20 17-18 18-19
19-20

exact/norm bonds :

1-2 1-6 2-3 2-12 3-4 3-14 4-5 4-11 16-17 16-20 17-18 18-19 19-20

exact bonds :

8-17 16-21

normalized bonds :

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isolated ring systems :

containing 1 :

G1:C,H

G2:S,N

Match level :

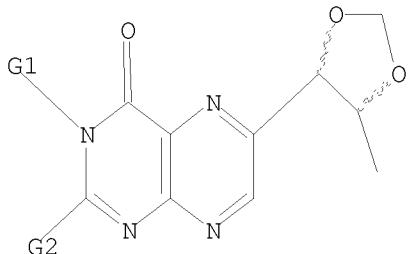
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11:CLASS 12:CLASS 14:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS

L3

STRUCTURE UPLOADED

10/513699

=> d 13
L3 HAS NO ANSWERS
L3 STR



G1 C,H
G2 S,N

Structure attributes must be viewed using STN Express query preparation.

=> s 13 full
FULL SEARCH INITIATED 14:34:07 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 19 TO ITERATE
100.0% PROCESSED 19 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.01

L4 6 SEA SSS FUL L3

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
SESSION
FULL ESTIMATED COST ENTRY 188.76 188.98

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FILE COVERS 1907 - 1 Mar 2009 VOL 150 ISS 10
FILE LAST UPDATED: 27 Feb 2009 (20090227/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

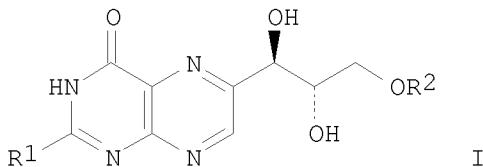
=> s 14 full
L5 5 L4

=> d ibib abs hitstr tot

L5 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2005:472157 CAPLUS
 DOCUMENT NUMBER: 143:7534
 TITLE: Preparation of tetrahydrobiopterin and analogs of tetrahydrobiopterin
 INVENTOR(S): Moser, Rudolf; Groehn, Viola; Schumacher, Andreas; Martin, Pierre
 PATENT ASSIGNEE(S): Biomarin Pharmaceutical Inc., USA; Merck Eprova A.-G.
 SOURCE: PCT Int. Appl., 55 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005049614	A2	20050602	WO 2004-US38313	20041117
WO 2005049614	A3	20070308		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004290692	A1	20050602	AU 2004-290692	20041117
CA 2545484	A1	20050602	CA 2004-2545484	20041117
EP 1776364	A2	20070425	EP 2004-819154	20041117
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, HR, LT, LV, MK, YU				
JP 2007534637	T	20071129	JP 2006-539994	20041117
US 20070244322	A1	20071018	US 2007-579106	20070216
PRIORITY APPLN. INFO.:			US 2003-520367P	P 20031117
			US 2003-520368P	P 20031117
			WO 2004-US38313	W 20041117

OTHER SOURCE(S): CASREACT 143:7534; MARPAT 143:7534
 GI



AB A process for the preparation of tetrahydrobiopterin and its analogs, e.g. I
 [R1 = alkylamino, arylamino, alkylthio, alkylaminomethyleneimino, R2 = H;
 R1 = alkylamino, alkylthio, Me2NCH:N, R2 = Me2CHET2Si, (Me3CO)Ph2Si,

MePh₂Si, Me₃CMe₂Si, Me₃C(MeO)PhSi, (Me₃C)₂MeSi, etc.], from neopterin and/or 6-substituted pterins with an improved yield and a high stereoselectivity is disclosed. Also disclosed herein are novel individual intermediates prepared in the preparation of tetrahydrobiopterin, such

as selectively protected neopterin useful for the preparation of tetrahydrobiopterin. As an example, L-neopterin was reacted with DMF-acetal to give the 2-(dimethylamino)methylene derivative I (R₁ = Me₂NCH₂:N, R₂ = H) (II). II was then silylated to I (R₂ = Me₃CPh₂Si) which could be deprotected to I (R₁ = NH₂).

IT 852547-48-9P

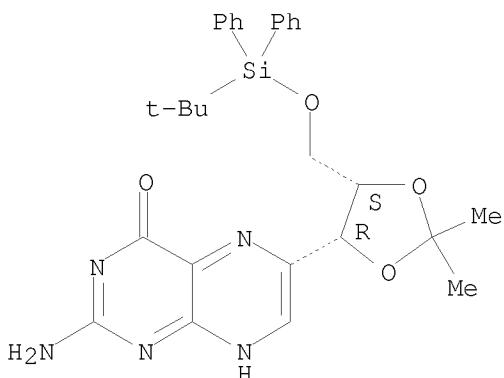
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of tetrahydrobiopterin and analogs)

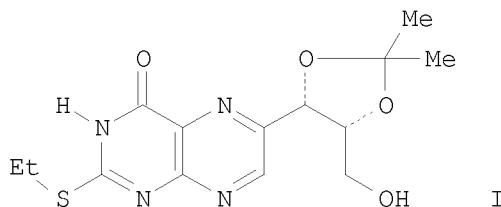
RN 852547-48-9 CAPLUS

CN 4(3H)-Pteridinone, 2-amino-6-[(4R,5S)-5-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2,2-dimethyl-1,3-dioxolan-4-yl]- (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2000:499841 CAPLUS
 DOCUMENT NUMBER: 133:207729
 TITLE: Synthesis of 2-ethylthio-6-(3-hydroxy-1,2-O-isopropylidenepropyl)pteridin-4(3H)-one
 AUTHOR(S): Kang, Yonghan; Kim, Seungjin; Myoung, Youngchan; Baek, Daejin
 CORPORATE SOURCE: Department of Chemistry, Hanyang University, Ansan, 425-791, S. Korea
 SOURCE: Heterocycles (2000), 53(7), 1551-1557
 CODEN: HTCYAM; ISSN: 0385-5414
 PUBLISHER: Japan Institute of Heterocyclic Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 133:207729
 GI



AB A strategy has been described for the synthesis of 2-ethylthio-6-(3-hydroxy-1,2-O-isopropylidenepropyl)pteridin-4(3H)-one (I), which can be used as a useful intermediate for the conversion of neopterin to biopterin.

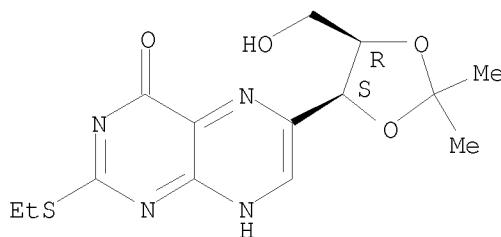
IT 290370-92-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (synthesis of 2-ethylthio-6-(3-hydroxy-1,2-O-isopropylidenepropyl)pteridin-4(3H)-one, a useful intermediate in the synthesis of biopterin)

RN 290370-92-2 CAPLUS

CN 4(3H)-Pteridinone, 2-(ethylthio)-6-[(4S,5R)-5-(hydroxymethyl)-2,2-dimethyl-1,3-dioxolan-4-yl]- (CA INDEX NAME)

Absolute stereochemistry.

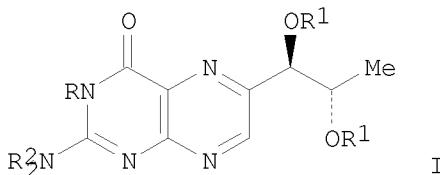


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17

THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

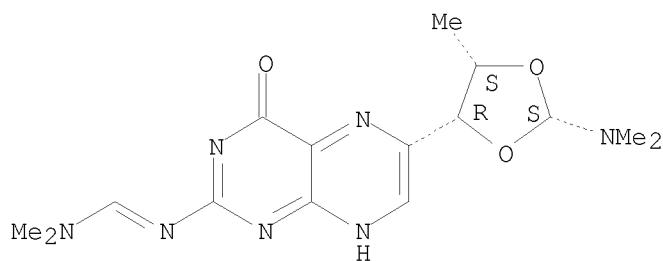
L5 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1995:536893 CAPLUS
 DOCUMENT NUMBER: 122:314347
 ORIGINAL REFERENCE NO.: 122:57165a, 57168a
 TITLE: Pteridines CV. Selective N(3)- and O4-alkylation of L-biopterin: A convenient synthesis of 3- and O4-methyl-L-biopterin and the versatile N2-(N,N-dimethylaminomethylene)-N(3)-p-nitrophenethyl-protected L-biopterin
 AUTHOR(S): Hanaya, Tadashi; Torigoe, Kiyoshi; Soranaka, Kazuyuki; Yamamoto, Horoshi; Qizheng, Yao; Pfleiderer, Wolfgang
 CORPORATE SOURCE: Faculty Science, Okayama University, Okayama, 700, Japan
 SOURCE: Pteridines (1995), 6(1), 1-7
 CODEN: PTRDEO; ISSN: 0933-4807
 PUBLISHER: International Society of Pteridinology
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Treatment of L-biopterin with N,N-dimethylformamide dimethyl- (or diethyl)acetal and then with acetic anhydride in pyridine gave 1',2'-di-O-acetyl-N2-(N,N-dimethylaminomethylene)-L-biopterin, which was converted by the Mitsunobu reaction into 3-Me and 3-p-nitrophenethyl derivs. The protective groups on the side chain diols and N2 of these compds. were selectively cleaved to furnish biopterins I (R = Me, R1 = H, R22 = CHNMe2; R = 4-O2NC6H4CH2CH2, R1 = H, R22 = CHNMe2; R = Me, 4-O2NC6H4CH2CH2, R1 = R2 = H), among which I (R = Me, R1 = R2 = H) is naturally occurring 3-methyl-L-biopterin and I (R = 4-O2NC6H4CH2CH2, R1 = H, R22 = CHNMe2) is N2,N(3)-protected biopterin, a versatile intermediate for various reactions on the side-chain diol. In contrast, the same Mitsunobu reactions of tri-N2:1',2'-O-acetyl-L-biopterin afforded O4-Me and O4-NPE derivs., both of which yielded O4-methyl-L-biopterin and subsequently led to 4-amino-L-biopterin.

IT 163132-77-2P 163252-46-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of alkyl biopterins)
 RN 163132-77-2 CAPLUS
 CN Methanimidamide, N'-[6-[2-(dimethylamino)-5-methyl-1,3-dioxolan-4-yl]-3,4-dihydro-4-oxo-2-pteridinyl]-N,N-dimethyl-, [2S-(2 α ,4 α ,5 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.

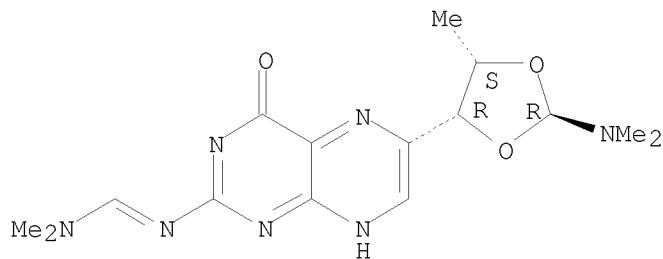


RN 163252-46-8 CAPLUS

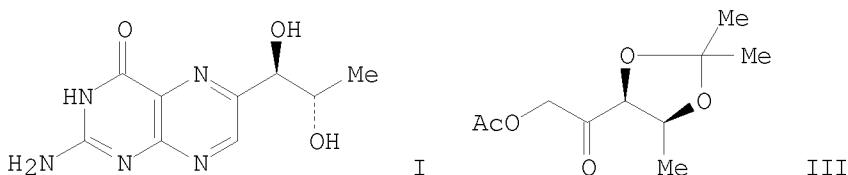
CN Methanimidamide, N'-[6-[2-(dimethylamino)-5-methyl-1,3-dioxolan-4-yl]-3,4-dihydro-4-oxo-2-pteridinyl]-N,N-dimethyl-, [2R-(2 α ,4 β ,5 β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.



L5 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1990:55443 CAPLUS
DOCUMENT NUMBER: 112:55443
ORIGINAL REFERENCE NO.: 112:9511a,9514a
TITLE: Synthesis of (-)-biopterin using (S)-ethyl lactate as
a starting material
AUTHOR(S): Kikuchi, Haruhiko; Mori, Kenji
CORPORATE SOURCE: Dep. Agric. Chem., Univ. Tokyo, Tokyo, 113, Japan
SOURCE: Agricultural and Biological Chemistry (1989), 53(8),
2095-100
CODEN: ABCHA6; ISSN: 0002-1369
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:55443
GI



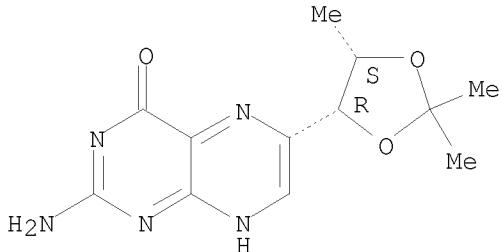
AB (-)-Biopterin (I) was synthesized from (1*S*,2*S*)-1-(1,3-dithian-2-yl)propane-1,2-diol (II), which was derived from com. available Et (*S*)-lactate. II was converted to ketone III through a six-step sequence. III was submitted to condensation with 3,5,6-triaminopyrimidinol, and followed by oxidation to afford isopropylidenebiopterin which was deprotected to give I.

IT 124600-40-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and
RN 124600-40-4 CAPLUS

CN 4 (1H)-Pteridinone, 2-amino-6-(2,2,5-trimethyl-1,3-dioxolan-4-yl)-, (4R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1972:126936 CAPLUS
 DOCUMENT NUMBER: 76:126936
 ORIGINAL REFERENCE NO.: 76:20553a,20556a
 TITLE: Pterin chemistry. 41. New synthesis of DL-biopterin
 AUTHOR(S): Viscontini, M.; Frei, W. F.
 CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, Switz.
 SOURCE: Helvetica Chimica Acta (1972), 55(2), 574-9
 CODEN: HCACAV; ISSN: 0018-019X

DOCUMENT TYPE: Journal
 LANGUAGE: German

AB D,L-Biopterin was prepared in .apprx.40% yield by condensing D,L-2,3-O-isopropylidene-4-methylerythrulose (I) with 2,4,5-triamino-6-hydroxypyrimidine, and oxidation with air to give D,L-1',2'-O-isopropylidenebiopterin. The isopropylidene protective group was easily hydrolyzed off to give isomer-free D,L-biopterin. I was prepared by oxidizing trans-crotonic acid to D,L-erythro-2,3-dihydroxybutyric acid, and introducing the protective group before the extra C.

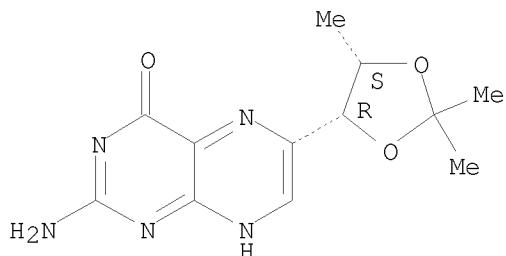
IT 36183-32-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 36183-32-1 CAPLUS

CN 4(3H)-Pteridinone, 2-amino-6-[(4R,5S)-2,2,5-trimethyl-1,3-dioxolan-4-yl]-,
 rel- (CA INDEX NAME)

Relative stereochemistry.



10/513699

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FULL ESTIMATED COST	29.20	218.18
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY	SESSION
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=> d his

(FILE 'HOME' ENTERED AT 14:30:02 ON 01 MAR 2009)

FILE 'REGISTRY' ENTERED AT 14:30:16 ON 01 MAR 2009
L1 STRUCTURE uploaded
L2 0 S L1
L3 STRUCTURE uploaded
L4 6 S L3 FULL

FILE 'CAPLUS' ENTERED AT 14:34:11 ON 01 MAR 2009
L5 5 S L4 FULL

FILE 'STNGUIDE' ENTERED AT 14:35:22 ON 01 MAR 2009

=> log y		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
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CA SUBSCRIBER PRICE	ENTRY	SESSION
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STN INTERNATIONAL LOGOFF AT 14:40:57 ON 01 MAR 2009